Nonlinear spin-polarized transport through a ferromagnetic domain wall

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A domain wall separating two oppositely magnetized regions in a ferromagnetic semiconductor exhibits, under appropriate conditions, strongly non linear I-V characteristics similar to those of a *p-n* diode. We study these characteristics as functions of wall width and temperature. As the width increases or the temperature decreases, direct tunneling between the majority spin bands reduces the effectiveness of the diode. This has important implications for the zero-field quenched resistance of magnetic semiconductors and for the design of a recently proposed spin transistor.

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It has recently been reported that some doped semiconductors, such as $Ga_{1-x}Mn_xAs$ [1] and $Ti_{1-x}Co_xO_2$ [2], undergo ferromagnetic transitions at temperatures as high as 110 K and 300 K respectively, while others (*n*-doped $Zn_{1-x}Mn_xSe$ [3]) are almost completely spin polarized by the application of a relatively modest magnetic field. These findings have raised hopes for the realization of semiconductor-based magnetoelectronic devices [4].

In a ferromagnetic semiconductor, the up- and down-spin components of just *one* carrier type are quite analogous to majority and minority carriers in ordinary doped semiconductors. Accordingly, a domain wall separating two ferromagnetic regions with opposite magnetizations is the analogue of a *p-n* junction, while two consecutive domain walls correspond to a *p-n-p* transistor. In a recent paper [5] we have exploited this analogy to show that nonlinear amplification of a spin-polarized charge current is indeed possible in the "*p-n-p*" configuration, and can be controlled by a magnetic field or a voltage applied to the "base" region between the two domain walls. However, the analysis of Ref. [5] was based on the assumption that the probability of a carrier flipping its spin while crossing the domain wall is negligible. This corresponds to assuming the resistivity of the domain wall is large compared to that of the bulk material.

The resistance of a domain wall between ferromagnetic materials has been examined several times from different perspectives since the pioneering work of Cabrera and Falicov [6]. These authors found that the resistance was very small, and later calculations [7, 8] have supported that result for metallic magnets. A far different regime is possible, however, when the spin polarization is or approaches 100%. For example, experimental and theoretical results[9] indicate that domain walls in $La_{0.7}Ca_{0.3}MnO_3$ may dominate the resistance in thin films. Magnetic semiconductor systems, due to their very small bandwidths, are also likely to be 100% spin polarized, and thus their domain walls should be highly resistive in the absence of spin-flip transport processes across them.

A key question that has not been addressed so far is how the nonlinear current-voltage (I-V) characteristics of the domain wall are affected by spin-flip processes as the width of the domain wall increases. Note that the width of a domain wall can now be directly measured [10] and, in principle, geometrically controlled [11]. Our analytical theory of transport across the domain wall should therefore be useful in designing devices with optimal values of the controllable parameters. Certainly such a theory would be crucial to understanding the zero-field quenched resistance and the low-field magnetoresistance of magnetic semiconductors as well as to the realization of the "unipolar spin transistor" proposed in [5].

Here we present a quantitative study of the nonlinear I-V characteristics of a magnetic domain wall. The main issue is the competition between minority spin injection, which is responsible for the nonlinear spin-diode behavior, and majority spin transmission, which tends to suppress it. We shall show that the latter dominates when either the temperature is low, or the domain wall is thick. Assuming that the motion of carriers through the domain wall is ballistic, we derive analytic expressions for the charge and spin currents as functions of applied voltage, width of the domain wall, and temperature. We further identify a new transport regime for intermediate wall thicknesses, in which carriers are ballistically transported across the domain wall (characterized by nonlinear charge currents), but most spin polarization is lost.

Our model is schematically depicted in Fig. 1(a). The two ferromagnetic regions $F1$ and $F2$ are connected by a domain wall region of width d, $-d/2 < x < d/2$. The exchange field $B(x)$ has the form

$$\vec{B}(x) = B_0[\cos\theta(x)\hat{x} + \sin\theta(x)\hat{y}], \qquad (1)$$

where $\hat{x}$, $\hat{y}$ are unit vectors in the direction of x and y, and the angle $\theta(x)$ varies linearly from $\theta = \pi/2$ in $F2$ to $\theta = -\pi/2$ in $F1$ [12].

We assume that d, while possibly large in comparison to a typical carrier wavelength, is smaller than the mean free path and the spin diffusion length L_s, which is in turn smaller than the geometric size of the system. A charge current J_q is injected from the left: our objective
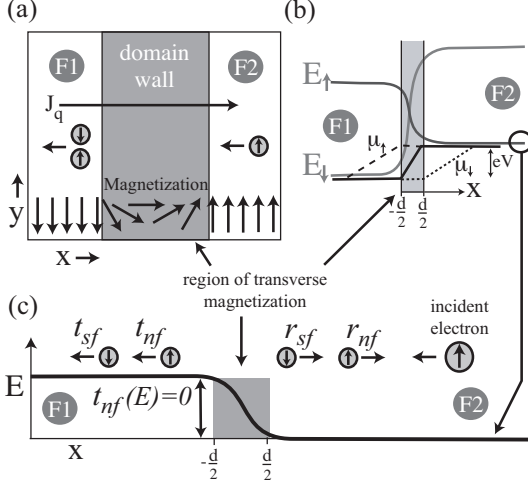
FIG. 1: (a) Schematic representation of a domain wall. (b) Qualitative behavior of the quasichemical potentials and the electrostatic potential (solid line). Note that the nonequilibrium voltage drop occurs within the interfacial region, while the nonequilibrium populations extend up to a distance of order L_s from it. (c) Reflection and transmission processes for an electron incident on the domain wall.

is to calculate the voltage V that develops across the domain wall and the spin current J_s due to the flow.

Let $\mu_>$ and $\mu_<$ be the quasi-chemical potentials, which control the nonequilibrium densities of majority and minority spin carriers respectively [13]. Far from the wall we have $\mu_> = \mu_<$ and the carrier densities have the equilibrium values $n_>^{(0)}$ and $n_<^{(0)}$, with $n_>^{(0)} >> n_<^{(0)}$. Density variations from equilibrium $\Delta n_{>(<)} \equiv n_{>(<)} - n_{>(<)}^{(0)}$ are related to the difference of the quasichemical potentials $\Delta \mu \equiv \mu_< - \mu_>$ near the domain wall. Since, by charge neutrality, $\Delta n_< \simeq -\Delta n_>$ we see that the *relative* change in the minority spin density is always much larger than the corresponding relative change in the majority spin density. This implies that $\mu_>$ is essentially pinned to its bulk value, while $\mu_<$ varies significantly in a region of length $\sim L_s$ on either side of the domain wall. We can therefore set $\mu_> \simeq 0$ throughout $F1$ and $\mu_> \simeq eV$ throughout $F2$, where V is the electrostatic potential of $F1$ relative to $F2$ (see Fig. 1(b)) and the carriers are assumed to be electrons. The density variations are

$$\Delta n_<(x) = n_<^{(0)} \left[e^{\Delta \mu(x)/k_B T} - 1 \right], \qquad (2)$$

where k_B is the Boltzmann constant and T is the temperature.

The charge currents for majority and minority spin orientations must satisfy the condition $J_> + J_< = J_q$ where the total charge current J_q is independent of position. In addition, the minority carrier current $J_<$ is almost entirely a diffusion current, and is given by the classical relation $J_<(x) = eD dn_<(x)/dx$, where D is the diffusion constant. Because the spin density relaxes to equilibrium exponentially on the scale of L_s (

i.e., $\Delta n_<(x) = \Delta n_<(\pm d/2)e^{-|x \mp d/2|/L_s}$ where the lower sign holds in $F1$ and the upper sign in $F2$), the minority carrier current at $x = \pm d/2$ can be written as $J_<(\pm d/2) = \mp eD\Delta n_<(\pm d/2)/L_s$, or, with the help of Eq. (2),

$$J_<(\pm d/2) = \mp \frac{eDn_<^{(0)}}{L_s} \left[e^{\Delta \mu(\pm d/2)/k_B T} - 1 \right]. \qquad (3)$$

It will be argued below that for nondegenerate carriers the quasi-chemical potential of minority spin electrons on each side of the domain wall adjusts to the quasichemical potential of majority spin electrons on the opposite side, so that $\mu_<(-d/2) \simeq eV$, $\mu_<(d/2) \simeq 0$ (see Fig. 1(b)), and

$$\Delta \mu(\pm d/2) = \mp eV. \qquad (4)$$

Under the same assumption of nondegeneracy, it will also be shown that the matching condition for the spin current $J_s(x) \equiv J_\uparrow(x) - J_\downarrow(x)$ is

$$\frac{J_s(-d/2)}{J_s(d/2)} = \frac{\bar{t}_- + \bar{t}_+ e^{-eV/k_B T}}{\bar{t}_+ + \bar{t}_- e^{-eV/k_B T}} \qquad (5)$$

where $\bar{t}_\pm = \bar{t}_{nf} \pm \bar{t}_{sf}$, and $\bar{t}_{sf}$ and $\bar{t}_{nf}$ are population-averaged transmission coefficients, with and without spin flip (see Fig. 1(c)), which will be defined more precisely below. Thus, the spin current is conserved across a sharp domain wall ($\bar{t}_+ = \bar{t}_-$), but reverses its sign across a smooth one ($\bar{t}_+ = -\bar{t}_-$).

Combining Eqs. (3-5), and using current conservation we arrive at our main results. First

$$\frac{J_q}{J_0} = \sinh\left(\frac{eV}{k_B T}\right) \left[1 + \frac{\bar{t}_{sf}}{\bar{t}_{nf}} \tanh^2 \left(\frac{eV}{2k_B T}\right) \right], \qquad (6)$$

where $J_0 \equiv 2eDn_<^{(0)}/L_s$. For $\bar{t}_{sf} = 0$ this reduces to the equation [14] derived in ([5]), while for $\bar{t}_{nf} = 0$ we get $V = 0$ as expected for a ballistic conductor. In the linear regime $eV/k_B T << 1$ this formula leads to the well-known interfacial resistance of Fert and Valet [15]. Second, in the immediate vicinity of the domain wall the spin current is given by

$$\frac{J_s}{J_0} = 2 \sinh^2 \left(\frac{eV}{2k_B T}\right) \left[1 \pm \frac{\bar{t}_{sf}}{\bar{t}_{nf}} \tanh \left(\frac{eV}{2k_B T}\right) \right], \qquad (7)$$

where the upper sign holds in $F2$ and the lower sign in $F1$. We see that spin-flip processes cause the appearance of an odd-in-voltage component of the spin-current, whereas, for $t_{sf} = 0$, the spin-current is an even function of V [5]. Shown in Fig. 2 is (a) the spin current in $F1$, (b) the charge current, and (c) the ratio of the two. The curves correspond to several different values of $\bar{t}_{nf}/\bar{t}_{sf}$. The trends for the spin and charge current described above are evident in Fig. 2; specifically the charge current is always odd in V whereas the spin current is even in the absence of spin-flip. When spin-flip
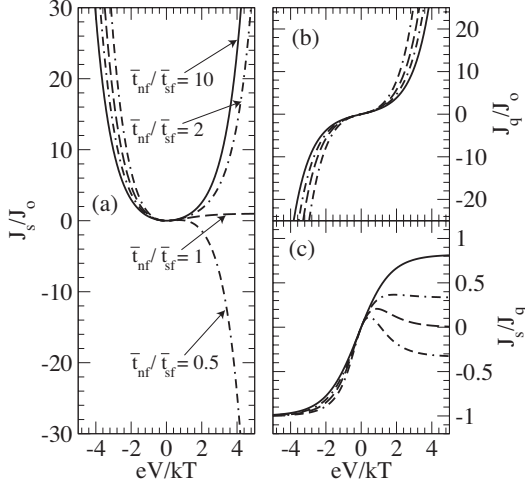
FIG. 2: (a) Spin current in $F1$, (b) charge current, (c) ratio of spin current to charge current vs. voltage for $\bar{t}_{nf}/\bar{t}_{sf} = 10,\ 2,\ 1,\ 0.5$.

dominates the spin current becomes odd as well. The spin current in $F2$ is related to that in $F1$ according to the following relation: $J_s(F2; V) = -J_s(F1; -V)$. As $\bar{t}_{nf}/\bar{t}_{sf}$ becomes smaller, the "leakage current" between the two majority bands becomes significant, and the odd in V term in the spin current begins to dominate. Over the entire range shown of $\bar{t}_{nf}/\bar{t}_{sf}$ the relationship between J_q and V is highly nonlinear indicating ballistic transport. Thus ballistic transport itself is not a sufficient condition for maintaining spin polarization in transport across a domain wall.

Assuming ballistic transport in the wall region, we calculate the transmission/reflection coefficients from the exact numerical solution of the Schrödinger equation

$$\left[\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - \frac{\Delta}{2} \begin{pmatrix} 0 & e^{-i\theta(x)} \\ e^{+i\theta(x)} & 0 \end{pmatrix} \right] \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} = E \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix},$$
(8)

where $\Delta = g\mu_B B$ is the exchange spin-splitting. The technique of solution is the same as used in Ref. [7]. Sample results are shown in Fig. 3(a)-(c) for three different values of the dimensionless parameter $\xi = \hbar\pi/2d\sqrt{2m\Delta} = 10$, 1, and 0.1, corresponding to sharp, intermediate, and smooth domain walls respectively. smooth domain walls respectively. Recent experiments [10] suggest the width of domain walls in artificial nanostructures can be as small as 1 nm, giving $\xi \sim 1$ for an effective mass m equal to the electron mass and a spin splitting $\Delta = 100meV$. Domain walls thinner than 20 nm have already been inferred in thin GaMnAs layers[16].

Fig. 3(d)-(f) shows the behavior of the key ratio $\bar{t}_{nf}/\bar{t}_{sf}$ as a function of temperature and thickness. As expected $\bar{t}_{nf}$ vanishes at low temperature, because, in this limit, there are no incident states above the exchange barrier to provide minority spin-injection. The spin diode is a thermally-activated device (as a p-n diode is), thus higher temperature is favorable to its performance. Fig.
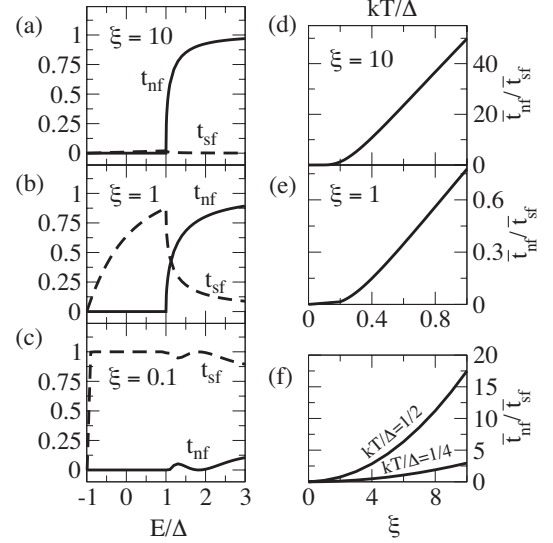

FIG. 3: (a)-(c) Energy dependence of transmission coefficients for $\xi = 10$, 1, and 0.1 respectively . (d)-(e) Ratio of the population averaged non-spin-flip to spin-flip transmission coefficients $(\bar{t}_{nf}/\bar{t}_{sf})$ vs. temperature for $\xi = 10$ and 1 respectively. (f) $\bar{t}_{nf}/\bar{t}_{sf}$ versus ξ for $k_B T/\Delta = 0.25$ and 0.5.

3(d,e) supports this view by showing that minority spin injection only dominates above a certain temperature (depending on domain wall thickness). However the condition $k_B T \lesssim \Delta$ must be respected if the system is to be nearly 100% spin-polarized. The conclusion is that there is a range $T_{min} < T < T_{max}$ in which unipolar spin diodes and transistors are expected to be operational.

We now come to the justification of the matching condition (5) and the calculation of the quasi-chemical potential offset. We begin with the former. In the spirit of the Landauer-Büttiker formalism we treat the ferromagnetic regions $F1$ and $F2$ as two reservoirs of spin polarized electrons at chemical potentials $\mu_1 = 0$ and $\mu_2 = eV$ which inject up- and down-spin electrons, respectively, in the domain wall region. The small density of minority spin carriers is neglected in the following argument. The components of the current due to electrons with energies in the range $(E, E + dE)$ on the two sides of the domain wall are given (in units of e/h) by

$$\begin{aligned} j_{1>}(E) &= -(1 - r_{nf}(E))f_{1>}(E) + t_{sf}(E)f_{2>}(E) \\ j_{1<}(E) &= r_{sf}(E)f_{1>}(E) + t_{nf}(E)f_{2>}(E) \\ j_{2>}(E) &= (1 - r_{nf}(E))f_{2>}(E) - t_{sf}(E)f_{1>}(E) \\ j_{2<}(E) &= -r_{sf}(E)f_{2>}(E) - t_{nf}(E)f_{1>}(E), \end{aligned}$$
(9)

where r_{nf} and r_{sf} are the non spin-flip and spin-flip reflection probabilities, related to t_{nf} and t_{sf} by the unitarity condition $r_{nf} + r_{sf} + t_{nf} + t_{sf} = 1$, and $f_{1>}$, $f_{2>}$ are shorthands for the equilibrium distributions of majority spin carriers in $F1$ and $F2$ respectively. Note that, for nondegenerate carriers $f_{1>} = f_{2>}e^{-eV/k_B T}$. We find that the spin-flip reflection coefficient r_{sf} is extremely small at all energies and thicknesses, and can

therefore be safely neglected. With this approximation, combined with the unitarity condition, it is easy to show that the energy-resolved currents are given by $j_{s1(2)}(E) = (t_{-(+)}(E) + t_{+(-)}(E)e^{-eV/k_BT})f_{2>}(E)$. Noting that $f_{2>}(E) \propto e^{-E/k_BT}$ and integrating over energy we see that the total current $J_{s1} = \int_0^\infty j_{s1}(E)e^{-e/k_BT}$ is equal to $A(\bar{t}_- + \bar{t}_+e^{-eV/k_BT})$ where the average transmission coefficients are defined as

$$\bar{t}_{nf(sf)} = \frac{\int_0^\infty t_{nf(sf)}(E)e^{-E/k_BT}dE}{\int_0^\infty e^{-E/k_BT}dE}, \qquad (10)$$

and A is a constant. Similarly $J_{s2} = A(\bar{t}_+ + \bar{t}_-e^{-eV/k_BT})$. The ratio J_{s1}/J_{s2} is thus given by Eq. (5).

To justify the quasi-chemical potential offset condition, Eq. (4) we notice that the quasi-chemical potential $\mu_{<,1}$ of minority spin electrons near the left hand side of the domain wall is an average of the quasi-chemical potentials of right (+) and left (-) moving electrons : $e^{\mu_{<,1}/k_BT} = [e^{\mu^+_{<,1}/k_BT} + e^{\mu^-_{<,1}/k_BT}]/2$. (A similar relation holds for the quasi-chemical potential $\mu_{<,2}$ of minority spin electrons near the right hand side of the domain wall). The quasi-chemical potentials for right and left movers on either side are determined by the conditions of continuity

$$
\begin{aligned}
e^{-(E-\mu^+_{>,2})/k_BT} &= qe^{-(E-\mu^+_{>,1})/k_BT} + pe^{-(E-\mu^+_{<,1})/k_BT} \\
e^{-(E-\mu^+_{<,2})/k_BT} &= qe^{-(E-\mu^+_{<,1})/k_BT} + pe^{-(E-\mu^+_{>,1})/k_BT} \\
e^{-(E-\mu^-_{<,1})/k_BT} &= qe^{-(E-\mu^-_{<,2})/k_BT} + pe^{-(E-\mu^-_{>,2})/k_BT} \\
e^{-(E-\mu^-_{>,1})/k_BT} &= qe^{-(E-\mu^-_{>,2})/k_BT} + pe^{-(E-\mu^-_{<,2})/k_BT},
\end{aligned}
$$
(11)

where $q = t_{sf}/(t_{sf} + t_{nf})$ and $p = t_{nf}/(t_{sf} + t_{nf})$ are the relative probabilities of transmission with and without spin flip respectively. The first of these equations, for example, says that the density of right-moving up-spin electrons of energy E on the right hand side of the domain wall is equal to the density of right-moving down-spin electrons of the same energy which enter from the left and flip their spin, *plus* the density of right-moving up-spin electrons which enter from the left and do not flip their spin. Because the quasi-chemical potentials of the majority spin carriers are essentially pinned to their bulk values, we can set $\mu^+_{>,2} = \mu^-_{>,2} = \mu_{>,2} = eV$ and $\mu^+_{>,1} = \mu^-_{>,1} = \mu_{>,1} = 0$. Integrating Eqs. (11) over energy, and making use of $p + q = 1$, we easily get $\mu_{<,1} = eV$ and $\mu_{<,2} = 0$, as indicated in Fig. 1(b).

In summary, we have shown that both the thickness and the temperature have a profound influence on the nonlinear transport properties of a ferromagnetic domain wall. We have derived analytical formulas, Eqs. (6) and (7), for the charge and spin currents of this "magnetic junction" under physical assumptions similar to the ones from which the Shockley equations of a classical *p-n* junction are derived. These formulae indicate a new transport regime, where charge transport is ballistic, but spin polarization is lost. Equations (6) and (7), together with microscopic calculation of the population-averaged transmission coefficients, can be used to assess the effectiveness of unipolar spin-diode devices in realistic circumstances.

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[13] The exact electronic states are, strictly speaking, neither "up" nor "down" with respect to the local magnetization, but superpositions of the two orientations. However, the relative phase of the up and down components of the wave function has a rapid spatial variation — typically on the scale of the electronic wavelength λ. Therefore transverse spin coherence disappears on a scale larger than λ, and the carriers' spin can be safely assumed to be either parallel or antiparallel to the local magnetization.
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